

Tellurium: An Extensible Python-based Modeling Environment for Systems and Synthetic Biology

Supplementary Materials

Kiri Choi[†], J Kyle Medley[†], Matthias König[‡], Kaylene Stocking[†], Lucian Smith[†], Stanley Gu[†], and Herbert M. Sauro^{†*}

[†]Department of Bioengineering, University of Washington, William H. Foege Building, Box 355061, Seattle, WA, USA, 98195-5061

[‡]Institute for Biology, Institute for Theoretical Biology, Humboldt University, Berlin, Germany

*Corresponding author

Parameter Estimation

To run the parameter estimation example, please obtain the benchmark suite (Villaverde et al., 2015) which will come with the model as well as the experimental data. Optimized parameters used to generate the figures are included in `parameter_fitting_result.csv` file.

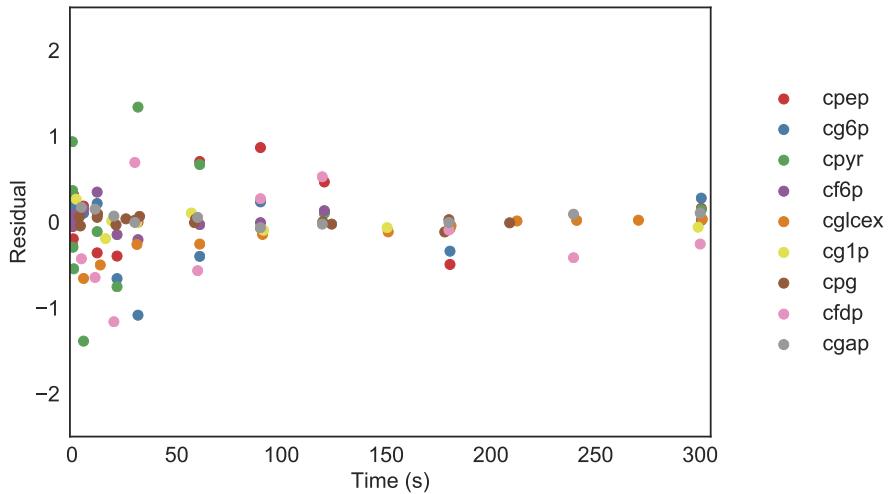


Figure 1: Residuals of central carbon metabolism model of *E. coli* fitted against experimental data of 9 metabolites.

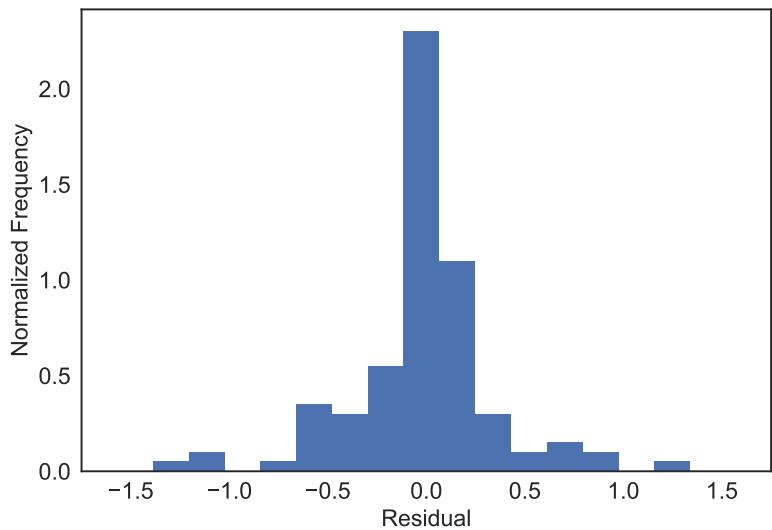


Figure 2: Normalized histogram of residuals of all data points combined.

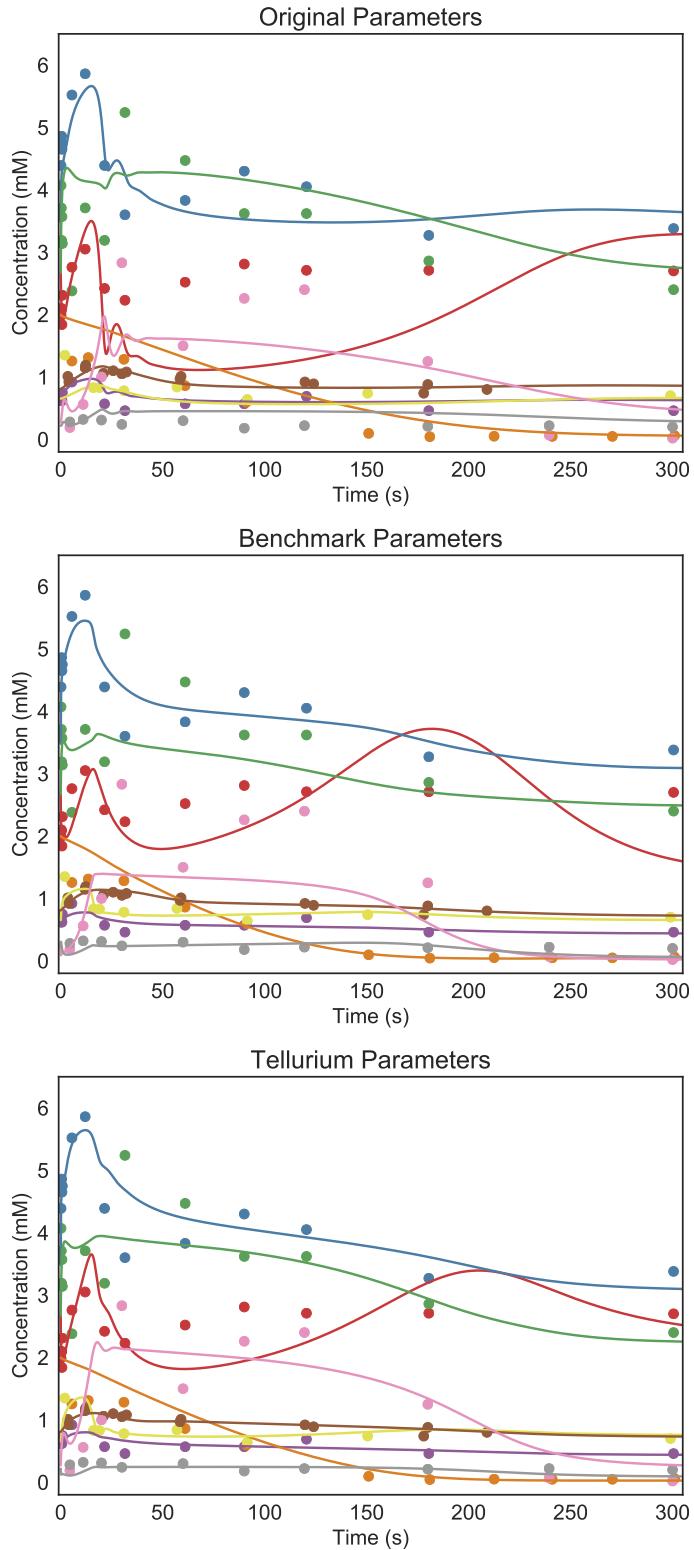


Figure 3: Comparison of fitted curves in parameter estimation example. From top to bottom: fitted curves using the original parameters, fitted curves using parameters from the benchmark suite, fitted curves using parameters from Tellurium. Lines represent simulated data using fitted parameters and dots represent the experimental data. Red, blue, green, purple, orange, yellow, brown, pink, and gray traces and dots corresponds to pep, g6p, pyr, f6p, glcex, g1p, pg, fdp, and gap, respectively.

Packages	Descriptions
libSBML	Library for working with SBML files (http://sbml.org/Software/libSBML)
libSEDML	Library for working with SED-ML files (https://github.com/fbergmann/libSEDML)
libCOMBINE	Library for working with COMBINE archives (https://github.com/sbmlteam/libCombine)
pySBOL	Library for working with SBOL files (https://github.com/SynBioDex/pysbol)
Antimony	Human-readable/writable representation of SBML (https://github.com/sys-bio/antimony)
phraSED-ML	Human-readable/writable representation of SED-ML (https://github.com/sys-bio/phrasedml)
simpleSBML	Library for simplifying model manipulation in libSBML (https://github.com/sys-bio/simplesbml)
libStructural	Library for structural analysis of network models (https://github.com/sys-bio/Libstructural)
libRoadRunner	Fast simulator supporting ODE and stochastic simulations, metabolic control analysis, and others (http://libroadrunner.org/)
AUTO2000	Library for bifurcation analysis (http://www.dam.brown.edu/people/sandsted/homcont.php)
COBRApy	Library for constraint-based modeling (https://opencobra.github.io/cobrapy/)
NumPy	Library for array-based computation (http://www.numpy.org/)
SciPy	Library for scientific computing (https://www.scipy.org/scipylib/index.html)
SymPy	Library for symbolic mathematics (http://www.sympy.org/en/index.html)
matplotlib	General 2D plotting library (https://matplotlib.org/)
seaborn	Statistical visualization library (https://seaborn.pydata.org/)
PySCeS	Library for simulations and structural analysis (http://pysces.sourceforge.net/)
CBMPy	Library for constraint-based modeling on PySCeS (http://cbmpy.sourceforge.net/)
PySB	Library for rule-based modeling (http://pysb.org/)
StochPy	Library for stochastic modeling (http://stochpy.sourceforge.net/html/userguide.html)
PySCeSToolbox	Library for metabolic control analysis on PySCeS (https://github.com/PySCeS/PyscesToolbox)

Table 1: Selected list of libraries included in Tellurium

References

Villaverde, A. F., Henriques, D., Smallbone, K., Bongard, S., Schmid, J., Cicin-Sain, D., Crombach, A., Saez-Rodriguez, J., Mauch, K., Balsa-Canto, E., et al., 2015. Biopredyn-bench: a suite of benchmark problems for dynamic modelling in systems biology. *BMC systems biology* 9 (1), 8.